1-Eicosanol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 362 °C

Global applicability domain: Inside

Local applicability domain index: 3.68e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

Image not found
1-Eicosanol
Measured: 372
Predicted: 362

Image not found
Heptadecan-1-ol
Measured: 333
Predicted: 331

Image not found
1-Hexadecanol
Measured: 334
Predicted: 324

Image not found
2,4,6-Tris(tert-butyl)phenol
Measured: 278
Predicted: 276